SECTION 2

QUESTION 1: Do the modeling frameworks used by USEPA include the significant processes affecting PCB fate, transport, and bioaccumulation in the Housatonic River; and are the descriptions of these processes in the modeling framework(s) sufficiently accurate to represent the hydrodynamics, sediment transport, PCB fate and transport, and PCB bioaccumulation in the Housatonic River?

2.1 GENERAL

The modeling frameworks presented in the MFD, which include the Hydrologic Simulation Program-Fortran (HSPF), the Environmental Fluid Dynamics Code (EFDC), and AQUATOX, account for the major processes affecting PCB fate, transport, and bioaccumulation within the Housatonic River. They are general modeling codes that contain equations describing a multitude of potentially important processes, including some that may not be significant to the long-term fate and bioaccumulation of PCBs.

The difficulty in any complex chemical fate, transport, and bioaccumulation modeling application is recognizing the relative importance of the different fate and transport mechanisms and focusing data collection and evaluation as well as the modeling efforts on those most relevant to the problem. As currently written, the MFD includes all conceivably relevant physical, chemical, and biological processes. The more difficult task of culling out the unimportant mechanisms has been postponed until later in the project.

Evaluation of the robust site-specific database and an *a priori* recognition of the most appropriate spatial and temporal scales are necessary to focus the model development process. Important decisions regarding the modeling framework, including selection of the model grid and development of a finalized list of relevant processes, have been largely postponed until later stages of the project.

2.2 CONCEPTUAL MODEL

The MFD presents a conceptual model developed from site-specific data. The data used to establish a conceptual model were limited to those collected by the Agency from 1998 to 2000. Prior historical data, as well as data collected by GE over the 1998 to 2000 time period, were not evaluated and integrated into the conceptual model. Evaluation of the complete site-specific data set can provide important insights into potentially relevant processes and assist in the evaluation of appropriate temporal and spatial scales in which to perform the mathematical modeling. Processes controlling the long-term fate of PCBs in the Housatonic River may not be evident in the temporally limited (1998 to 2000) data set presented in the MFD. For example, natural recovery processes such as burial of sediment PCB deposits by relatively clean tributary solids cannot be assessed by examining a temporally limited data set. Long-term temporal trends in surface sediment, water column, and fish concentrations represent the most effective means of evaluating the nature and magnitude of the natural recovery process. Additionally, by limiting the data considered for conceptual model development to the 1998 to 2000 time period, it is impossible to evaluate the consistency of the conceptual model across different integration periods and media. Since the conceptual model forms the basis for the mathematical model, it should be developed and tested against the entire data set, especially since long-term simulations will be used for mathematical model calibration and predictions.

2.2.1 Processes Included in the Conceptual Model

The conceptual model presented in the MFD identifies a number of important fate and transport processes, including (MFD page 3-52):

- partitioning of PCBs to organic carbon and sediments,
- non-partitioning of PCBs (presence of PCBs in free non-aqueous-phase liquid (NAPL–*i.e.,* oil),
- diffusion to the water column,
- bed load transport,

- advection (from groundwater to surface water), and
- bioturbation.

2.2.2 Overview of Relevant Processes

The conceptual model presented in the MFD does not provide the detail needed to evaluate the approaches to be used to model a number of potentially relevant processes. For example, there is no discussion of how PCB partitioning to sediment particles will be modeled. Will sorption to inorganic solids be accounted for and, if so, how? The "non-partitioning of PCBs" presumably refers to the behavior of an oil phase. The MFD does not discuss how such a phase would be modeled. How will transport of this phase and dissolution kinetics be handled? Volatilization was not included as a significant PCB fate process; however, no data were presented that support the exclusion of this process. What is the basis for excluding volatilization? What equations will be used to describe it if it is to be included? Volatilization may be a significant process, particularly within the quiescent backwater regions, and should be included in the modeling framework.

The MFD makes numerous statements regarding the importance of different PCB fate processes based on very limited data, and in some instances suspect data and dubious data evaluation. This includes the discussion of:

- PCB distribution,
- sequestration of PCBs,
- sediment erosion,
- water column and sediment partitioning,
- non-partitioning of PCBs (e.g. PCB NAPLs),
- sediment bed load,
- wind-driven transport of particulates within Woods Pond,
- bioturbation, and
- dating of sediment deposits.

These processes are discussed in the following sections.

2.2.3 PCB Distribution

Summaries of sediment PCB concentrations by depth (MFD, Table 3-9 and Table 3-11) are presented as a means to interpret the vertical distributions of PCBs within the system. This analysis could lead to erroneous conclusions because it improperly aggregates disparate data. For example, the averages presented in Table 3-9 were computed from samples throughout the study reach and thus do not take into account the documented strong spatial concentration gradient in which higher PCB concentrations are located nearer the source. As a result, the average concentrations presented for the various depth increments do not reflect any differences in vertical distribution that may be affected by their distance form the source. This analysis also ignores the differences in the number and location of samples used to calculate the averages for the various sediment depths. As such, the depth comparison mixes regions of the River which may be undergoing significant net deposition with those that may be undergoing net erosion. Finally, the data charts do not present any estimate of variance. Simple examination of mean concentrations is inadequate to evaluate the vertical trends in the data. For example, a limited number of high PCB concentrations at the surface of Woods Pond sediments may produce an elevated mean concentration relative to underlying sediments, when in fact a majority (or some) of the sediment cores may not reflect this vertical distribution. This improper aggregation of disparate data could lead to the erroneous conclusion that PCBs are not being sequestered anywhere within the Pond.

2.2.4 Sequestration of PCBs

The MFD cites a lack of strong vertical gradients in sediment PCB concentrations as evidence that PCBs are not being sequestered via burial (MFD page 3-57; Table 3-9). The apparent presumption is that net burial would be evidenced by a positive gradient of PCB concentration with depth below the sediment surface. However, this presumption would only be true if PCB concentrations on water column particulate matter have undergone the significant decline necessary to produce a vertical gradient in sediments at locations where sediments are accumulating. The MFD provides no discussion of this issue. Further, the interpretation of gradients is confounded by the fact that the analyses rely on dry weight-based data integrated over different sediment types and locations. Sequestration of PCBs should be assessed from vertical patterns examined on a core-by-core basis to differentiate spatial differences in sediment composition and deposition rates.

Moreover, the appropriate basis for comparison of PCB concentrations is on an organic carbon-normalized basis. PCBs are hydrophobic. As such, they preferentially associate with organic matter within the sediments. Consequently, sediments containing high organic matter content typically contain higher PCB concentrations than sediments with low organic content. To account for this general phenomenon, the spatial distribution of sediment PCBs should be examined on an organic carbon-normalized basis. This will account for the influence that the horizontal and vertical distribution in sediment organic matter has on total dry weight PCB concentrations.

2.2.5 Sediment Erosion

The MFD presents the decline of PCB concentration between the East Branch/West Branch confluence and Roaring Brook and the subsequent increase to Woods Pond as evidence of erosion (MFD page 3-57). This is misguided. First of all, dry weight-based spatial patterns are confounded by the strong longitudinal gradient in sediment organic matter content. This is clear when the dry weight concentration gradient is compared with the organic carbon-normalized concentration gradient. The organic carbon-normalized gradient is continuous and shows no evidence of an increase as one proceeds downstream. In addition, the MFD ignores the influence of dilution on the spatial gradients. In the Housatonic River, as in all other contaminated sediment sites, concentrations decline as one progresses downstream from the source due to dilution by the water and particulate matter that enters from tributaries and direct drainage. Erosion removes PCBs from sediments, but its effect on PCB concentration is dependent on the vertical concentration patterns and the depth to which erosion had progressed at the time of sampling. In short, while erosion may be occurring within the reach in question, spatial patterns in dry weight PCB concentrations cannot be used as evidence of its occurrence.

2.2.6 Water Column PCB Partitioning

The water column partitioning data suggest that the measurements may be spurious (MFD page 3-65). The data indicate tremendous variation in the particulate-phase concentration that appears to be independent of the dissolved-phase concentrations. For example, four of the samples had dissolved concentrations that were nearly identical (*i.e.,* range from 14 to 17 ng/L) and little variation in TSS (*i.e.,* range from 1.3 to 3.4 ppm). In contrast, particulate-phase PCB concentrations in these samples varied by a factor of almost 700 (*i.e.,* range from 0.5 ppm to 340 ppm). For all the data, the dissolved PCB concentration ranged over a factor of 6 (*i.e.,* 14 to 83 ng/L), whereas the particulate concentration ranged over a factor of almost 2000 (*i.e.,* 0.5 ppm to 910 ppm). The problems with the water column partitioning data likely result from the small sample volumes (*i.e.,* 1 liter). Dissolved-phase PCBs may have sorbed onto the filter and glassware and corrupted the separation of the dissolved and particulate phases. These data should not be used to specify water column partitioning. Additional sampling and analysis utilizing large volume samples (16-20 liters), as originally specified in the USEPA Housatonic River Work Plan (Weston, 1999), should be collected, filtered, and analyzed for dissolved and particulate-phase PCB congener concentrations. The larger volumes will minimize the effects of glassware and filter surfaces on water column partition coefficients.

2.2.7 Non-Partitioning of PCBs

The MFD suggests that PCBs may be present in a “third phase,” presumably an oil phase, within the sediments (MFD page 3-52 and 3-65). PCBs have been observed in such a phase during the removal of sediments from the upper 0.5 mile reach of the River near the GE plant site. The evidence presented in the MFD for a sediment oil phase containing PCBs includes the depressed two-phase sediment PCB partition coefficients (K_d) and the lack of correlation between sediment TOC and PCB concentration, as well as sediment grain size and PCB concentrations within the upstream reach of the study area.

The K_d values presented in the MFD simply represent the total sediment PCB concentrations divided by total PCB concentrations within extracted sediment pore water. Log

K_d values ranged from 2.2 to 3.9. In contrast, the log K_{ow} for Aroclor 1260, the predominant Aroclor found within the system, is approximately 6.3. The depressed log K_d values relative to the K_{ow} for the source Aroclor may be due to a number of factors, including incomplete sediment pore water separation and/or dissolved organic carbon (DOC) effects in the pore water, as discussed below.

Incomplete sediment pore water separation would have produced elevated pore water PCB concentrations relative to those expected by equilibrium partitioning. Was good and consistent separation of bulk sediments and sediment pore waters achieved?

The K_d values exhibit a spatial pattern that is inconsistent with the concept that oil may be controlling pore water PCB concentrations within the upper reaches of the study area. The K_d values are lowest downstream of river mile (RM) 130 where sediment grain sizes are smaller and sediment TOC concentrations are higher than near the plant site. The average K_d value at RM 130 and above is about 3700. The average K_d value below RM 130 is about 600. If oil were controlling the pore water concentration, the K_d values should be lower in the large grain-size and low-TOC sediments located upstream of river mile 130. The opposite is true.

The spatial pattern in K_d values may also be controlled by DOC within the pore waters. DOC can have a profound effect on pore water PCB concentrations, particularly for the higher chlorinated congeners with high organic carbon partition coefficients (K_{oc}). For a log DOC partition coefficient (K_{doc}) of 5.0, pore water DOC concentrations of 10 and 100 mg/L would increase sediment pore water PCB concentrations by 2 and 11 times, respectively, over pore water containing no DOC. Considering the spatial pattern in sediment TOC, it is likely that pore water DOC concentrations are higher in the sediments in the downstream region of the study area. This may have produced the spatial pattern in K_d values.

Considering that only 11 samples have corresponding sediment pore water and total PCB measurements, additional sediment PCB partitioning studies should be conducted. Sediment partitioning is an important parameter controlling such processes as benthic invertebrate PCB exposure and sediment-water PCB exchange. Therefore, additional sampling and analysis should be conducted to constrain this parameter in the modeling effort.

The lack of correlation between sediment TOC and PCB concentrations within the region of the River near the plant site is an interesting observation. The MFD suggests that a sediment PCB phase other than that partitioned onto organic carbon may be responsible for this phenomenon (MFD Figure 3-18). However, correlations of such parameters as PCBs and TOC are sensitive to imprecisions in the analytical methods. This may be particularly important considering the low levels of TOC and high levels of PCBs observed in the upper portions of the study area. Additional data analysis is warranted to further explore the potential impact that analytical precision in TOC and PCB measurements has on the PCB/TOC correlation. Can the lack of correlation be wholly or partially explained by the imprecision of TOC and PCB measurements at the concentrations observed near the plant site? This can be examined by evaluating the field duplicate TOC and PCB data collected from that reach.

Additionally, the high-flow water column particulate and dissolved-phase PCB measurements do not support the existence of a significant oil phase within the sediments. Sampling conducted during high flows demonstrates that the majority of PCBs present in the water column are associated with the suspended particulates (MFD page 3-72). If oil containing PCBs were present in significant quantities within the surface sediments, then water column dissolved-phase PCB concentrations would likely represent a significant fraction of the total PCB within the water column during high-flow events that produce sediment scour. However, the lack of detection of dissolved-phase PCBs during the storm events may be influenced by limitations of the sampling and analytical procedures, as discussed above.

Since the development of the MFD, the USEPA has conducted scanning electron microscope (SEM) and x-ray defraction (XRD) analyses on numerous sediment samples from the upper portion of the study area that exhibit high PCB concentrations, large grain size, and low organic matter content (USEPA, unpublished data). These analyses have indicated that the chlorine content (presumably PCBs) of these samples is often associated with an organic coating on the larger grain-size (sand) particles within the samples. Although qualitative in nature, these data may explain the elevated PCB concentrations exhibited by these sediments as well as the observed spatial patterns in K_d values and the high-flow water column PCB partitioning data discussed above, which (as noted) are inconsistent with a hypothesized PCB oil phase within the sediments. In short, insofar as the SEM/XRD analyses suggest that PCBs are present on large inorganic particles in the form of an organic coating, they do not support the presence of a separate PCB oil phase, but they do indicate that the transport of the larger inorganic particles in the upstream reach of the study area plays a significant role of the fate of PCBs within the reach.

2.2.8 Sediment Bed Load

The MFD at several points mentions sediment bed load transport as a potentially important process that will be modeled (MFD pages 3-52, 3-61, 3-65). Further, the recent SEM/XRD analyses suggest that sediment PCBs may be associated with organic coatings on coarse-grained sediment particles that predominate in the upper portion of the study reach (see Section 2.2.7 above). The presence of PCBs as a coating on coarse-grained sediment particles elevates the importance of sediment bed load as a transport mechanism for the non-cohesive sediments within the River. Currently, no direct measures of sediment bed load have been made within the Housatonic River, nor does the MFD present any plans for collection of such data. Sediment bed load measurements should be made from a number of locations within the study area, with focus on Reach 5A, including the model boundary. Reach 5A sediments are coarser, and consequently more subject to sediment bed load processes, than the downstream reaches. Moreover, accurate specification of the sediment bed load boundary condition is critical to modeling this process, particularly considering the coarse grain size and elevated PCB concentrations observed within the reach of the River located upstream of the proposed model boundary.

2.2.9 Wind-Driven Transport of Particulate PCBs

The MFD notes that wind may affect sediment distribution in Woods Pond via wind-driven transport of floating solids and suspended plant material, as suggested by the elevated PCB concentrations along the shoreline in areas that are not adjacent to submerged sediments with similarly elevated concentrations (MFD page 3-59). However, the latter observation is not evidence that wind-driven transport of particulate matter to the shoreline is a significant process. PCB concentrations may be higher near the shoreline due to a lack of burial or the sediment transport and deposition characteristics of the pond, independent of wind-driven transport. What additional efforts is the USEPA conducting to further evaluate wind-driven PCB transport in Woods Pond? Wind-driven transport would add substantial complexity to the modeling effort. Wind-driven transport should not be included in the modeling framework unless unequivocal data are generated to demonstrate that this process is occurring.

2.2.10 Bioturbation

The MFD indicates that the process of bioturbation is important in determining PCB fate and transport, including both suspended solids transport and sediment bed load transport (MFD page 3-48). Bioturbation impacts the rate of mixing of surficial sediments and thereby influences the surficial sediment PCB concentration in contact with surface waters. Accordingly, bioturbation influences PCB diffusive exchange and the rate of natural recovery. The former is affected by the replenishment of surface sediment PCBs through the mixing of deeper sediment segments with those at the sediment surface. The latter is affected by mixing subsurface PCBs with clean solids depositing on the surface. Typically, bioturbation is controlled by the macroinvertebrate population. Sediment mixing induced by macroinvertebrate activity typically extends to between 5 and 10 cm into the sediments (Boudreau, 1998; Thoms *et al*., 1995). The MFD suggests that bioturbation may be influenced by the feeding and spawning activities of carp. The MFD mentions that a bioturbation study will be conducted to further evaluate this process. However, no details of the study are provided. Any assessment of bioturbation should be focused on quantifying its effects on surface sediment mixing at the spatial scale of the model. Gradients, or lack thereof, in such parameters as Pb^{210}, PCBs, and bulk density within the surficial 15 cm of the sediment can be used as a means of assessing the depth and intensity of sediment mixing. Many of these data have been collected in recent years by GE and the USEPA. Anecdotal information such as the observation of sediment plumes during carp feeding activity cannot be used to quantify sediment bioturbation. Additionally, population estimates alone cannot accurately assess the influence of such activity on the sediments. The assessment of bioturbation should be based on a direct measure of its effects on surface sediment physical and chemical profiles.

2.2.11 Dating Sediment Deposits

The MFD confuses Pb^{210} and stable Pb in its discussion of the use of radiotracers to date sediment deposits (MFD page 3-19). The MFD incorrectly indicates that Pb^{210} dating is based on locating the depth at which concentrations drop and assuming that that drop coincides with the drop in atmospheric Pb concentrations that occurred in the 1970s. In fact, it is a drop in concentrations of stable Pb, not Pb^{210}, in sediment cores that can provide an indication of the sedimentation rate, due to the substantial decline in stable Pb deposition rates since the reduction in leaded gasoline use in the 1970s. In contrast to stable Pb, Pb^{210} is a daughter product of radium. Pb^{210} profiles can also be used to date sediment deposits, but the analysis is more complicated than simple visual inspection of sediment profiles as is conducted using stable Pb data. Pb^{210} is produced by the atmospheric decay of U^{238}, has a half-life of 22 years, and has a relatively constant deposition rate. By applying this half-life and deposition rate information, gradients in Pb^{210} can be used to estimate sediment age. The vertical profile of Pb^{210} can also be used to develop an understanding of the depth of active biological mixing. Sharp vertical gradients in the surficial sediment are indicative of low-intensity mixing while a lack of vertical gradient in Pb^{210} is indicative of active mixing.

2.3 WATERSHED MODELING (HSPF)

Watershed processes will be simulated using the Hydrological Simulation Program–FORTRAN (HSPF) model. This model has been developed and used during approximately the last 20 years. Numerous watershed studies have been conducted using HSPF and the model has been applied to a wide range of drainage basins throughout the country. This model is supported by USEPA.

All significant watershed processes are incorporated into HSPF. As noted in the MFD (page 4-2), this model will be applied to the Housatonic River watershed to provide the following: 1) water balance; 2) solids balance; 3) PCB loading; and 4) nutrient loading. Generally, HSPF's descriptions of processes controlling watershed-scale transport of water, solids, and nutrients are sufficiently accurate to meet the modeling objectives. However, site data are insufficient to parameterize and calibrate PCB loadings from the watershed.

Watershed PCB loadings are derived from a number of potential sources, including atmospheric deposition, groundwater, and surface water runoff. Insufficient data exist to parameterize HSPF for these different sources. Hence, the modeling effort will need to rely on a number of assumptions, including PCB concentrations in precipitation, in groundwater, and on surface soil particles. These assumptions may affect the response of watershed PCB loadings to year-to-year changes in climatic conditions, thereby adding considerable uncertainty to the long-term projections. Considering the inherent uncertainties in these assumptions, HSPF should not be used to develop watershed PCB loadings. Rather, the existing data should be used directly to establish the appropriate concentrations to specify at the model boundaries. The uncertainties associated with specifying PCB boundary conditions can then be explored through appropriate alternative PCB fate model simulations using different, yet credible, boundary conditions.

2.4 HYDRODYNAMIC, SEDIMENT TRANSPORT AND ABIOTIC PCB FATE MODELING (EFDC)

The Environmental Fluid Dynamics Code (EFDC) will be used to simulate hydrodynamics, sediment transport, and abiotic PCB transport in the Housatonic River. Similar to HSPF, this model is supported by USEPA and has a long history of development and application. The hydrodynamics of a wide range of rivers, estuaries and coastal ocean regions have been modeled using EFDC, which was originally developed as a hydrodynamic model. Sediment transport, contaminant fate, and eutrophication modeling capabilities have been added to EFDC during approximately the last five to ten years.

The hydrodynamic submodel incorporates all significant physical processes controlling the movement of water in the River. The difficulty with the Housatonic River, as noted in the MFD (page 4-19), will be applying this model so that computationally feasible simulations can be realized while providing sufficient accuracy to address PCB fate and transport issues. The MFD focuses on relatively fine-scale temporal and spatial processes that might not significantly impact PCB transport processes at scales important to the system as a whole and to ecological and human health risk. As an example, the MFD describes the development of a three-dimensional hydrodynamic model of Woods Pond based on observed thermal stratification during low-flow periods in the summer (MFD page 3-45). While stratification does occur in portions of Woods Pond during low-flow periods, it is unclear whether these stratification processes significantly impact PCB fate and transport in the River. It is quite possible that including three-dimensional transport processes in the modeling framework is not necessary for accurate simulation of PCB fate over the spatial and temporal scales of importance in this study.

The sediment transport component of EFDC includes a wide range of formulations to simulate suspended load transport of cohesive and non-cohesive sediments, bed load transport, and related bed mechanics. The sediment transport formulations incorporated into EFDC have been used in numerous studies and, generally, this submodel incorporates all significant processes. However, several potential problems exist with the approach presented in the MFD. First, bed load transport is mentioned several times in the report, but few details are provided concerning: 1) specific formulations to be used, 2) methods and data to determine boundary conditions (e.g., incoming bed load at upstream boundary), 3) methods to calibrate and validate the bed load submodel, and 4) methods to incorporate bed load fluxes in the PCB fate models. Second, simulating non-cohesive bed armoring may be problematic. The MFD states (page 4-26) that the van Rijn (1984) formulation will be used if bed armoring is included in the model. The van Rijn (1984) method does not simulate bed armoring. In EFDC, only the Garcia and Parker (1991) method simulates bed armoring, but it is inappropriate for the Housatonic River modeling due to differences in the dominant grain sizes for which it was formulated and those which exist within the Housatonic River. Finally, as noted above, EFDC contains a wide range of formulations to simulate cohesive and non-cohesive sediment transport processes. The MFD has not sufficiently specified which formulations will be used in the Housatonic River study, so it is difficult to determine the adequacy of the Agency's approach. The USEPA should consider using the van Rijn (1984) method for simulating the suspended load transport of non-cohesive sediments. In addition, the bed armoring procedure developed by van Niekerk *et al*. (1992), or a variant of that method (QEA 1999), should be used in conjunction with the van Rijn (1984) formulations.

The MFD also states (page 4-26) that depth-dependent erosion rates and critical shear stress measurements needed for input to EFDC will be obtained from sediment erosion data collected using a device called a Sedflume. This device has been used to study the erosion properties of sediments from several other riverine systems, including the Lower Fox River in Wisconsin and the Grand River in Michigan (McNeil, 1996; Lick, 1999). Sedflume measures gross erosion rate as a function of depth in the bed over a shear stress range of 1 to about 100 dynes/cm^2. Critical shear stress cannot be measured directly with Sedflume; it can only be inferred by assuming that the shear stress at which an arbitrarily low erosion rate (typically, 10^{-4} cm/s) occurs corresponds to the critical shear stress. Even though Sedflume experiments may produce interesting and useful data for the Housatonic River, these data are not directly applicable for use in the EFDC sediment transport model. In fact, there is no publicly available model to which Sedflume data can be applied. Special modifications to the erosion formulations in EFDC will need to be made because Sedflume provides information on gross erosion rate, not net erosion rate, which is needed in a sediment transport model. Sedflume data can be used to provide insights into the erosion properties of Housatonic River sediments. However, if USEPA attempts to use Sedflume erosion rate data in the current version of EFDC, the model will significantly over-predict resuspension.

The abiotic PCB transport submodel includes many of the important processes controlling the fate of PCBs in the Housatonic River. However, the MFD suggests (page 3-52) that sediment bed PCBs may be associated with a "third phase," likely oil. As discussed in Section 2.2.7, the currently available data do not support the presence of a significant PCB oil phase within the sediments. However, to the extent that USEPA intends to address this additional phase, the contaminant transport submodel in EFDC does not include formulations that describe the transport or dissolution of oil-phase chemicals. Additional model code development would be required to simulate these processes within EFDC.

2.5 BIOTIC PCB FATE AND PCB BIOACCUMULAITON MODELING (AQUATOX)

AQUATOX is a modeling framework that has been under development for more than 25 years. USEPA is currently supporting its use and further development. AQUATOX simulates processes relating to the dynamics of ecological communities (changes in the biomass of species), eutrophication, as well as the fate and transport, bioaccumulation, and toxicological impacts of xenobiotic chemicals. The MFD indicates (Section 4.2.3) that USEPA intends to use all of these capabilities of AQUATOX, except for the assessment of toxicological impacts.

AQUATOX incorporates many of the important PCB fate and bioaccumulation processes, including water flows, solids transport, chemical partitioning, volatilization, and dechlorination. As noted above, the MFD suggests that there is evidence that some PCBs in the sediments are associated with an undefined phase, likely oil (MFD pages 3-52 and 3-65). AQUATOX does not include equations to describe the transport or dissolution of oil-phase PCBs. To the extent that USEPA wishes to assess this additional phase within the overall PCB fate and transport modeling, additional formulations will be needed in AQUATOX.

Probably the most important issue associated with the use of AQUATOX in the Housatonic River project is that many of the processes simulated by the model cannot be tested or calibrated because of a lack of site-specific data. This applies particularly to the computation of population densities of invertebrates and fish (in units of biomass; g/m2), about which very little is known for the Housatonic River. At most, a snapshot of measured values concerning invertebrate and fish densities will be available. This is insufficient to assess model performance, as the densities of natural animal populations are notoriously variable throughout a given year and from year to year.

In addition, the equations depicting biomass are over-simplified representations of complex ecological processes. The biomass of a species can change in response to food availability as well as other factors, including competition, predation, disease, habitat changes, and variation in year class strength (determined primarily in the first two years of life; Wootton, 1990; Kramer and Smith, 1962). These factors are either not modeled or are represented simplistically, so that the realism of the average computed biomass and year-to-year variation in biomass cannot be assessed.

The biomass predictions by themselves will apparently not be used for making risk management decisions. However, they may affect decision-making insofar as they may affect the PCB bioaccumulation calculations. PCB concentrations in fish are controlled, in part, by the pathway by which they are transferred to the fish, that is, the food web. In AQUATOX, the food web is specified as a set of feeding preferences for each species that are modified according to prey availability. Thus, even if a forage fish has a strong preference for water column plankton, if the biomass model computes a severe reduction in the plankton biomass, then the fish may actually consume predominantly benthic invertebrates. However, the dynamics of prey availability computed by AQUATOX will not be adequately constrained by site data, since sufficient data do not exist. Therefore, the PCB exposure source to the fish may change depending on prey availability. In this way, the predictions of the bioaccumulation model will be unconstrained and thus highly uncertain, and yet that uncertainty will not be explicitly recognized.

A more realistic approach is to bound the diet of each species based on the available site data and published studies in other water bodies, and then to calibrate the model by adjusting the diets within these bounds. Because of the uncertainty in the diets, it will be necessary to explore the sensitivity of the model results to alternative diets that are consistent with the available natural history information.